

Dynamics of Holes and Universality Class of the Antiferromagnetic Transition in the Two Dimensional Hubbard Model

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The dynamics of a single hole (or electron) in the two dimensional Hubbard model is investigated. The antiferromagnetic background is described by a Néel state, and the hopping of the carrier is analyzed within a configuration interaction approach. Results are in agreement with other methods and with experimental data when available. All data are compatible with the opening of a mean field gap in a Fermi liquid of spin polarons, the so called Slater type of transition. In particular, this hypothesis explains the unusual dispersion relation of the quasiparticle bands near the transition. Recent photoemission data for $\text{Ca}_2\text{CuO}_2\text{Cl}_2$ are analyzed within this context.

The nature of the insulating phase of the Hubbard model in a bipartite (square) lattice has attracted a great deal of attention. A clarification of the universality class of the transition will greatly help in understanding the nature of the “metallic”, gapless, phase away from half filling. A detailed discussion of the issue can be found in [1]. Opposing viewpoints on the problem are presented in [2,3]. An appealing approach is the scaling analysis discussed in [1]. It is assumed that physical quantities can be expressed in terms of a single energy scale, Δ , which vanishes at the transition. A wealth of numerical results suggest that such scaling does exist. The data implies that typical length scales, ξ , scale as $\Delta^{-\frac{1}{4}}$. This implies the existence of a quasiparticle band, in the gapless side, with a dispersion relation $\epsilon_k \propto k^4$ [4,5].

The understanding of the Mott transition as function of filling in the Hubbard model in two dimensions (2D) requires a knowledge of the dynamics of carriers introduced into the undoped antiferromagnetic (AF) system. This problem has been studied in the related t - J model [6,7]. The bands obtained by numerical methods are well described within the Born approximation [8], which accounts for hopping in one sublattice only. It has been shown that higher order corrections are small [9,10]. The bandwidth scales, approximately, with $J = 4t^2/U$. This can be understood from the fact that a spin flip is required to restore the AF background to its original texture after a hole hops between equivalent sites. Numerical results for the Hubbard model [11,12], show similar features, with a narrow band which is very flat between the $(0, \pi)$ and $(\pi/2, \pi, 2)$ points of the Brillouin Zone. This band is also reasonably described by a generalization of the Born approximation to the Hubbard model [13]. As for the t - J model, this picture suggest that numerical results are well described in terms of dressed holes which hop within a given sublattice.

The same picture is obtained from mean field calculations. It has been shown that single holes in the Hubbard model induce the formation of inhomogeneous spin tex-

tures [14], which can be described as spin polarons, or spin bags [15]. An improved wavefunction results from hybridization of polarons localized at different sites, so that the translational symmetry is restored [16]. This is a standard procedure in molecular physics, where Hartree-Fock (HF) solutions are improved by the Configuration Interaction (CI) method. The resulting polaron band is in reasonable agreement with other calculations [17,18].

In the following, we analyze the implications of the spin polaron band of the simple Hubbard model for the nature of the Mott transition. We also extend these calculations to include second and third nearest neighbor hoppings, in order to compare directly to experiments [19,20]. Our results suggest that a mean field picture is a reasonable starting point for the analysis of the dynamics of holes in the Hubbard model in 2D, providing an intuitive picture of the Mott transition, and reproducing adequately the main features observed in the experiments.

The usual HF approximation to the Hubbard model with nearest neighbor couplings only in a square lattice, gives an AF ground state at half filling. This solution reproduces the existence of a gap in the charge excitations, which scales with U , for large U . The approximation misses the low energy spin waves, which can be incorporated by including the low amplitude fluctuations around the local minimum defined by the HF solution, that is, the Random Phase Approximation (RPA). The RPA reproduces the correct result in the large U limit [15,21]. Thus, the mean field solution is a good starting point for the analysis of the hole dynamics.

A naive generalization of the AF solution to the doped case can be obtained by filling the lowest lying states in the upper Hubbard band. Fig. 1 shows this (HF) band in the extended Brillouin Zone, for $t = 0.35$ eV and $U = 3.92$ eV, in order to compare to experiments (see below). Due to the AF background, the bands have an additional periodicity, so that the point (π, π) is degenerate with $(0, 0)$. As the Hubbard model in the absence of other hoppings has electron-hole symmetry, the same

band describes electrons. The HF band shows a flat dispersion along the $(0, \pi) \rightarrow (\pi/2, \pi/2)$ direction. The HF band can be written in the extended zone scheme as:

$$\epsilon_k = \frac{\Delta}{2} - \sqrt{\frac{\Delta^2}{4} + 4t^2[\cos(k_x) + \cos(k_y)]^2} \quad (1)$$

where $\Delta = \frac{U}{2}\langle n_\uparrow - n_\downarrow \rangle$. Near the upper edge, this band can be approximated by: $\epsilon_k \approx (4t^2/\Delta)[\cos(k_x) + \cos(k_y)]^2$. It describes a hole with effective hoppings t^2/Δ to the neighbor in position $(2, 0)$, and $2t^2/\Delta$ to that at $(1, 1)$. Hopping between different sublattices is not allowed. Around the point $(0, \pi)$, we can expand: $\epsilon_k \approx (t^2/\Delta)(k_x^2 - k_y^2)^2$. This quartic dispersion explains well the findings reported in [4,5].

The integrated density of states is dominated by the flatness of the dispersion around $(0, \pi)$. Integrating over \vec{k} , we find, in the Hartree Fock case, $D(\omega) \sim \log[t^2/(U\omega)]/\sqrt{\omega}$ near the upper band edge, and a similar dependence for the polaron band.

The state $\tilde{c}_{k,\uparrow}^\dagger |\Psi_0\rangle$, where $|\Psi_0\rangle$ is the Slater determinant which describes the AF insulator, has negative compressibility and is unstable against charge inhomogeneities [14]. This topic was first discussed in [22]. As the compressibility, κ , is proportional to $(\partial\mu/\partial n)^{-1}$, it will be negative if the chemical potential is lowered upon doping [23]. The states near the gap edges are almost perfectly localized in one sublattice or the other. Thus, the additional electrons reduce the value of $\langle n_\uparrow - n_\downarrow \rangle$ by an amount directly proportional to the density. The gap is lowered by $\frac{Un}{2}$, where n is the hole density per lattice site. Because of the singularity in the density of states at the gap edge, the difference between the chemical potential and the gap edge increases as $\delta\mu \propto n^2$, neglecting logarithmic corrections. This dependence cannot compensate the decrease in the gap, $\propto n$, and the chemical potential is lowered upon doping. The transverse spin susceptibility also shows an instability as a consequence of the singularity in the density of states. Note, however, that the flatness of the band, which is a typical precursor of ferromagnetism [24], does not imply a ferromagnetic instability. The interaction between carriers of opposite spin is greatly reduced, as they are localized in different sublattices. This analysis is in agreement with general studies of the possibility of phase separation in the Hubbard model [22]. Similar results can be rigorously demonstrated in the limit of infinite dimensions [25].

The previous shortcoming of the homogeneous mean field solution of the doped Hubbard model can be overcome by considering generic charge and spin textures [14]. Among the many different solutions which are extrema of the Hartree Fock solutions, spin polarons and domain walls tend to be the most stable. We now analyze in detail the spin polaron, which is more stable at large values of U/t , and its energy is further lowered by delocalization effects (see also below). The spin polaron, in the

large U limit, can be approximately described as a self localized electron (or hole) for a cluster which contains at least five sites, and with a ferromagnetic alignment of the spins in its interior. The overlap between this solution and homogeneous solutions decays with the size of the cluster as $1/L^2$ [26], implying the formation of a localized state. This state is separated from the upper (lower) Hubbard band by an energy of order t in the large U limit. This splitting suppresses the contribution of the extra electrons to the spin susceptibility, curing the instabilities of the homogeneous HF approximation. In addition to this state, another localized level splits off from the lower (upper) band, and moves to an energy of order of a fraction of U from that band. Thus, the low energy spectral weight per electron (hole) is greater than one, in qualitative agreement with the arguments given in [27]. The Slater determinant which describes a solution of this type can be written as:

$$|\Psi_i\rangle = \tilde{c}_{i,\uparrow}^\dagger \Pi_i \left(\sum_k \alpha_k^i \tilde{c}_{k,s}^\dagger \right) \left(\sum_{k'} \beta_{k'}^i \tilde{c}_{k',s} \right) |\Psi_0\rangle \quad (2)$$

where $|\Psi_0\rangle$ describes the antiferromagnetic insulator at half filling. Thus the wavefunction $|\Psi_i\rangle$ is obtained from $|\Psi_0\rangle$ by adding a given number of electron-hole excitations, plus an electron (hole) at site i .

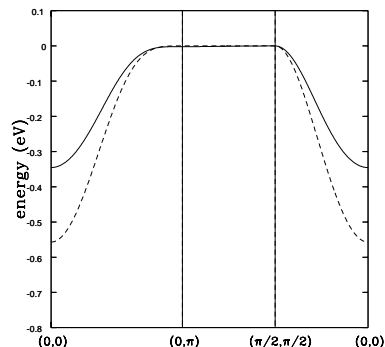


FIG. 1. Quasiparticle band structure for a single hole in the Hubbard band with $t = 0.35\text{eV}$ and $U = 3.92\text{eV}$. Hartree-Fock approximation: dashed line. CI approximation (full line): dispersion relation, see Eq. (3), fitted to the numerical results for a 14×14 cluster.

As discussed elsewhere [17,18], corrections to this inhomogeneous HF solution can be of two types: low amplitude fluctuations, which can be studied within the RPA [28], and hybridization of solutions centered at different lattice sites [16]. The combination of these solutions leads to wavefunctions of the type $|\Psi_k\rangle = \sum_i e^{i\vec{k}\cdot\vec{r}_i} |\Psi_i\rangle$, and to the formation of a polaron band, whose width scales as t^2/U in the limit of large U .

The dispersion band for a 14×14 cluster and the same values of U and t used above, is shown in Fig. 1. The

polaron (CI) band has the same shape than the HF band but is substantially narrower (around a 40%). We ascribe this narrowing to the fact that the polaron band is more strongly dressed by spin excitations (note, however, that the approximation used here only includes longitudinal, Ising like, modes). Because of the extension of the individual polarons, the band cannot be parametrized in terms of a few hopping parameters, as in the homogeneous solutions described previously. The numerical results of Fig. 1 can be accurately fitted by,

$$\epsilon_{\mathbf{k}} = \epsilon_0 + 4t_{11} \cos(k_x) \cos(k_y) + 2t_{20} [\cos(2k_x) + \cos(2k_y)] + 4t_{22} \cos(2k_x) \cos(2k_y) + t_{31} [\cos(3k_x) \cos(k_y) + \cos(k_x) \cos(3k_y)] + 2t_{40} [\cos(4k_x) + \cos(4k_y)]. \quad (3)$$

with $t_{11} = 0.130542$ eV, $t_{20} = 0.062056$ eV, $t_{22} = -0.006130$ eV, $t_{31} = -0.003963$ eV, and $t_{40} = -0.000836$ eV. In the $(0, \pi - \eta)$ direction we can expand the dispersion relation for small η as,

$$\epsilon_{\mathbf{k}} \approx \epsilon_0 + 4(-t_{11} + t_{20} + t_{22} - 2t_{31} + t_{40}) + 2\eta^2(t_{11} - 2t_{20} - 4t_{22} + 10t_{31} - 8t_{40}) + \frac{\eta^4}{3}(-\frac{1}{2}t_{11} + 4t_{20} + 8t_{22} - 41t_{31} + 64t_{40}). \quad (4)$$

Using the parameters given above we obtain $\epsilon_{\mathbf{k}} \approx -0.004\eta^2 + 0.08\eta^4$. This result shows that the quartic term dominates, as in HF and in agreement with [4,5].

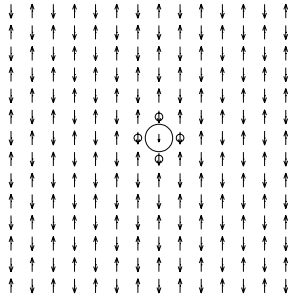


FIG. 2. Spin (arrows) and charge distribution around a localized hole in a 14×14 cluster using the parameters from Ref. [20].

Experiments on the dynamics of holes in CuO planes suggest that a Hubbard model with nearest neighbor hoppings only is insufficient [29,19,20]. The inclusion of additional hoppings is straightforward within the scheme discussed here. We have calculated the electron and hole bands using the parameters given in [20]: $U = 3.92$ eV, $t = 0.35$ eV ($J = 0.125$ eV), $t' = -0.12$ eV and $t'' = 0.08$ eV. For hole doping this choice of parameters leads to the formation of well localized spin polarons at the mean field level. The spin and charge textures associated to the (hole) spin polaron are shown in [2], for a 14×14 cluster.

We find no inhomogeneous solutions for electron doping (see below)

The quasiparticle bands are shown in fig.[3]. The new hoppings break the electron-hole symmetry present in the simple Hubbard model and induce a quadratic dispersion at the band edges, which dominates the quartic terms discussed so far. This dispersion relation implies that, upon doping, emptying the lowest lying states give a change in the chemical potential $\delta\mu \propto n$ that can be compensated by the decrease in the gap $\propto n$. As a result, homogeneous mean field solutions can be stable. The HF and CI bands have a similar shape, while, as in the case of the simple Hubbard model, the CI band is much narrower than the CI band (an approximate reduction of 40% is noted). As remarked in [20] the HF band is much wider than the one given by photoemission experiments. The CI band is in much closer agreement with the observed band (approximately 0.4 eV wide) and with the numerical results for the corresponding t - J model reported in [19]. The shape of the hole band shown in Fig. 2 is also in full agreement with experiments. The CI band can be fitted with the dispersion relation of Eq. (3). In this case the parameters are $t_{11} = -0.071428$ eV, $t_{20} = 0.195491$ eV, $t_{22} = -0.016190$ eV, $t_{31} = 0.003486$ eV, and $t_{40} = -0.006278$ eV. The expansion near $(0, \pi)$ gives constant $-0.63\eta^2 + 0.05\eta^4$, which is mainly quadratic.

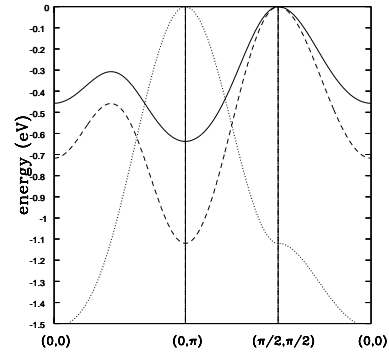


FIG. 3. Quasiparticle band structure for a singly doped Hubbard model with second and third nearest neighbor hoppings, using the parameters from Ref. [20] Hartree-Fock approximation: dashed line (hole doping) and dotted line (electron doping). CI approximation (full line): dispersion relation, see Eq. (3), fitted to the numerical results for a 14×14 cluster.

A detailed analysis of the hole dispersion relation in the corresponding $t - t' - t'' - J$ model is presented in [30]. It is instructive to compare our results with those there. As mentioned at the beginning, the nature of the approximation used here for the Hubbard model describes similar processes to those included in the Self Consistent Born Approximation used in [30]. However, when reducing the Hubbard hamiltonian to the t - J one, hopping terms $\propto J$

are neglected. Thus, the bandwidth obtained from the $t - J$ hamiltonian should be smaller than the exact. The approximation used here neglects the interaction of the hole with transverse spin waves, which probably leads to an overestimation of the exact bandwidth. Magnetic correlations around the hole are in qualitative agreement with [30] (see fig.[2]).

For electron doping, instead, the homogeneous solution is stable. The HF band is shown in Fig. [3]. The band has a significantly smaller effective mass near $(0, \pi)$ than in the case of hole doping, in agreement with [19], resulting in a larger quasiparticle peak as observed experimentally [19].

The instability of the homogeneous mean field solution for the doped Hubbard model can also lead to the formation of stripes, or domain walls [14,31–33]. Similar solutions have been found in the $t-J$ model [34,35]. A transition from the undoped insulator to a doped system with stripes should be qualitatively different from the one described above. The stripes will remain, most likely, static, even after the inclusion of corrections beyond HF. The lack of long range magnetic order can be understood from the weakening of the effective exchange coupling, and the enhancement of fluctuations [36], as for the spin polaron solutions. Thus, we cannot rule out the possibility of a sharp discontinuity, as function of U/t and for a fixed low doping, between a gapless phase with delocalized spin polarons, and another with static domain walls.

The above analysis shows that the properties of the insulating and the lightly doped phases of the Hubbard model can be reasonably understood within straightforward extensions of mean field theory. The picture is similar to the spin bag model [15,37,38]. The main difference is that the spin bag approach uses homogeneous solutions as starting point. We have addressed the instabilities of these solutions, and showed how they can be overcome. The adequacy of mean field theory in describing the metal-insulator transition is due to the suppression of dynamic charge fluctuations by the formation of the staggered magnetization, as in infinite dimensions [39]. The resulting picture leads to a flat quasiparticle band, in agreement with detailed numerical calculations. The density of states is singular at the band edges, enhancing the effects of the interactions. A quartic dispersion relation is obtained around the point $(0, \pi)$. Including second and third nearest neighbors hoppings allows us to compare with recent photoemission data. This new hoppings enhance the quadratic terms in the dispersion relation and break the electron/hole symmetry. The CI hole band is much narrower than the HF band and in agreement (both shape and width) with the experimental results.

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